A numerical approach to infrared divergent multi-parton phase space integrals

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It is described how the method of sector decomposition can serve to disentangle overlapping infrared singularities, in particular those occurring in the calculation of the real emission part of $e^+e^- \to 2\,$jets and $e^+e^- \to 3\,$jets at NNLO.

1. INTRODUCTION

Particle physics nowadays has largely become a matter of high precision measurements, which on the theory side requires an increasing number of loops and legs to be included in the calculations.

The process $e^+e^- \to\,$jets is particularly interesting, from an experimental as well as a theoretical point of view, because of its "clean" initial state, such that it can serve for a very accurate determination of α_s. However, LEP experiments already have shown that theoretical predictions at next-to-leading order (NLO) are not always sufficient to match the experimental precision [1], and this of course will be even more true for a future Linear Collider.

These facts have triggered a lot of progress in the calculation of NNLO corrections in recent years [2]. The last missing piece for the construction of an NNLO Monte Carlo program for the process $e^+e^- \to 3\,$jets is in fact the double real radiation part, which involves phase space integrations over five partons, where up to two of them can become unresolved, leading to infrared singularities.

The conventional way to deal with these singularities is to establish a subtraction scheme to isolate the divergent part [3,4,5]. The latter then is calculated analytically in $D = 4 - 2\epsilon$ dimensions, leading to $1/\epsilon$ poles which will cancel against the ones from the virtual corrections. This proce-

dure has been applied very successfully in NLO calculations. Its generalization to NNLO however is far from being straightforward. Nevertheless, subtraction schemes have been proposed in the literature [6,7,8,9,10], whereas the problem of integrating the subtraction terms analytically in D dimensions has been solved only for the case $e^+e^- \to 2\,$jets so far [11,12,8].

What will be suggested here is a new method which does not rely on explicit subtraction terms. The infrared singularities are isolated in an automated way using sector decomposition [13,14]. The cancellation of the pole coefficients with the ones from the virtual corrections can be verified numerically. The method already has been applied successfully to the process $e^+e^- \to 2\,$jets [12,15,16,17].

2. SECTOR DECOMPOSITION

The method of sector decomposition acts on parameter integrals and serves to factorize singularities which have an overlapping structure, as in the following simple example:
$I = \int_0^1 dx_1\, dx_2\, x_1^{-1-\epsilon}\, [x_1 + x_2]^{-1}$. Decomposing the parameter space into two sectors where the integration variables are ordered and remapping the integration range to the unit square factorizes the singularity:

$$I = \int_0^1 \frac{dx_1\, dx_2}{x_1 + x_2}\, x_1^{-1-\epsilon}\, [\underbrace{\Theta(x_1 - x_2)}_{(1)} + \underbrace{\Theta(x_2 - x_1)}_{(2)}]$$

The substitution $x_2 = x_1 t_2$ in sector (1) and $x_1 = x_2 t_1$ in sector (2) leads to

$$
\begin{aligned}
I \;=\; & \int_0^1 dx_1\, x_1^{-1-\epsilon} \int_0^1 dt_2\, (1+t_2)^{-1} \\
& + \int_0^1 dx_2\, x_2^{-1-\epsilon} \int_0^1 dt_1\, t_1^{-1-\epsilon}\, (1+t_1)^{-1} \;.
\end{aligned}
$$

For more complicated functions, this procedure may have to be iterated, but the principle is simple and easily automated. This is particularly true for multi-loop integrals because they have, after Feynman parametrization and integration over the loop momenta, the following universal form (L is the number of loops, N the number of propagators and D the space-time dimension)

$$
\begin{aligned}
G \;=\; & (-1)^N \Gamma(N - LD/2) \int_0^\infty \prod_{j=1}^N dx_j \qquad (1) \\
& \delta\Big(1 - \sum_{i=1}^N x_i\Big) \frac{\mathcal{U}(\vec{x})^{N-(L+1)D/2}}{\mathcal{F}(\vec{x}, \{s, m^2\})^{N-LD/2}} \;,
\end{aligned}
$$

where $\mathcal{U}$ and $\mathcal{F}$ are polynomials in the Feynman parameters and $\mathcal{F}$ also contains kinematic invariants. Applying the sector decomposition algorithm [14] to loop integrals in the form (1) isolates the dimensionally regulated poles in terms of factorizing Feynman parameters. Then subtractions of the singularities are carried out, using identities like

$$
\begin{aligned}
& \int_0^1 dx_1\, x_1^{-1+\kappa\epsilon} \mathcal{F}(x_1, \hat{x}) \\
& = \frac{1}{\kappa\epsilon} \int_0^1 dx_1\, \mathcal{F}(x_1, \hat{x})\, \delta(x_1) + \\
& \int_0^1 dx_1\, x_1^{-1+\kappa\epsilon} \left[\mathcal{F}(x_1, \hat{x}) - \mathcal{F}(0, \hat{x}) \right] , \qquad (2)
\end{aligned}
$$

where $\hat{x} = x_2, \ldots, x_N$ and $\lim_{x_1 \to 0} \mathcal{F}(x_1, \hat{x})$ is finite by construction, such that the second term in (2) is a plus distribution:

$$
\begin{aligned}
& \int_0^1 dx_1\, x_1^{-1+\kappa\epsilon} \left[\mathcal{F}(x_1, \hat{x}) - \mathcal{F}(0, \hat{x}) \right] \\
& = \sum_{n=0}^\infty \frac{(\kappa\epsilon)^n}{n!} \int_0^1 dx_1 \left[\frac{\ln^n(x_1)}{x_1} \right]_+ \mathcal{F}(x_1, \hat{x}) \;.
\end{aligned}
$$

Doing these subtractions for all x_i results in a Laurent series

$$
\mathcal{I} = \sum_{k=-2L}^b \epsilon^k C_k + \mathcal{O}(\epsilon^{b+1}) \;,
$$

where the order b of expansion in ϵ is in principle only limited by CPU time. However, the pole coefficients C_k being sums of complicated parameter integrals, their analytical evaluation is in general impossible. Therefore they are integrated numerically. For multi-loop integrals involving more than one kinematic invariant, Euclidean points have to be chosen in order to have stable numerics. In this way, results have been obtained [18] for example for massless 2-loop 4-point functions with 2 off-shell legs, where no analytical results exist yet, all 4-point master integrals needed for the calculation of 2-loop Bhabha scattering with massive fermions (analytical results exist for two of them [19,20,21]), two-point-functions with 4 and 5 loops, and for the planar massless 3-loop 4-point-function with on-shell legs calculated analytically by V.A. Smirnov [22].

3. PHASE SPACE INTEGRALS

The phase space integration for the production of N massless particles $q \to p_1, \ldots, p_N$ can be written as

$$
\begin{aligned}
& \int d\Phi_{1\to N} = (2\pi)^{N-D(N-1)} \\
& \int \prod_{j=1}^N d^D p_j\, \delta^+(p_j^2) \delta\Big(q - \sum_{i=1}^N p_i\Big) \\
& = (2\pi)^{N-D(N-1)}\, 2^{1-N} \\
& \int \prod_{j=1}^{N-1} d^{D-1}\vec{p}_j\, \frac{\Theta(E_j)}{E_j}\, \delta^+\big([q - \sum_{i=1}^{N-1} p_i]^2\big) \;.
\end{aligned}
$$

At this point one could pick a particular frame and integrate over energies E_j and angles θ_j, but for our purposes it is more convenient to integrate over the scaled invariants s_{ij}/q^2, $s_{ij} = (p_i + p_j)^2$, because in this way the singularities are located at the origin of parameter space and no particular axis is preferred. The transformation to the

integration variables

$$x_1 = s_{12}/q^2, x_2 = s_{13}/q^2, x_3 = s_{23}/q^2,$$
$$x_4 = s_{14}/q^2, x_5 = s_{24}/q^2, x_6 = s_{34}/q^2, \ldots$$

introduces a Jacobian which is proportional to the square root of the determinant of the Gram matrix $G_{ij} = 2p_i p_j$. The phase space then takes the form[2]

$$\int d\Phi_{1\to N} = C_\Gamma^{(N)}(q^2)^{(N-1)D/2-N} \int \prod_{j=1}^{n_s} dx_j$$

$$\delta(1 - \sum_{i=1}^{n_s} x_i)\Big[\Delta_N(\vec{x})\Big]^{\frac{D-(N+1)}{2}} \Theta(\Delta_N) \qquad (3)$$

$$n_s = N(N-1)/2$$
$$\Delta_N = |\det G|\,(q^2)^{-N}$$
$$C_\Gamma^{(N)} = (2\pi)^{N-D(N-1)} 2^{1-ND/2}$$
$$\times V(D-1)\ldots V(D-N+1)$$
$$V(D) = 2\pi^{\frac{D}{2}}/\Gamma(\frac{D}{2})\,.$$

3.1. $1 \to 4$ phase space

As an example, let us consider the integration of some squared matrix element $|M_4|^2$ over the $1 \to 4$ partonic phase space, relevant for the calculation of $e^+e^- \to 2\,\text{jets}$ at NNLO:

$$\int d\Phi_{1\to 4} = C_\Gamma^{(4)}(q^2)^{3D/2-5}$$

$$\int \prod_{j=1}^{6} dx_j\, \delta(1 - \sum_{i=1}^{6} x_i)\,|M_4|^2$$

$$[-\lambda(x_1 x_6, x_2 x_5, x_3 x_4)]^{-1/2-\epsilon}\,\Theta(-\lambda) \qquad (4)$$

$$\lambda(x,y,z) = x^2 + y^2 + z^2 - 2\,(xy + xz + yz)\,.$$

The matrix element is of the form

$$|M_4|^2 \sim \frac{\mathcal{P}_1(\vec{x}, \epsilon)}{(x_2 + x_4 + x_6)(x_3 + x_5 + x_6)x_4}$$
$$+ \frac{\mathcal{P}_2(\vec{x}, \epsilon)}{x_2(x_2 + x_4 + x_6)^2} + \ldots ,$$

---

[2]Note that for $N \geq 6$ $\det G$ is zero for 4-dimensional momenta because, after elimination of p_6 by momentum conservation, the vectors p_1 to p_5 will still be linearly dependent. Therefore we only consider the case $N < 6$ here.

where the $\mathcal{P}_k(\vec{x}, \epsilon)$ are some polynomials in the variables x_i. We again see the sums of Feynman parameters in the denominator, corresponding to triple invariants s_{ijk}, giving rise to an overlapping structure. Therefore, the form of the integral (4) is very similar to the one in eq. (1) for loop integrals and the overlapping singularities can be disentangled by the same principle. However, there are also very important differences to loop integrals. The most important one consists in the fact that in phase space integrals, non-polynomial structures (square roots) appear. For example, solving the constraint $-\lambda > 0$ in (4) for x_6 leads to $x_6^- < x_6 < x_6^+$ with $x_6^\pm = (\sqrt{x_2 x_5} - \sqrt{x_3 x_4})^2/x_1$. The substitution $x_6 \to (x_6^+ - x_6^-)\,y_6 + x_6^-$ remaps the integration range of x_6 to an integral from 0 to 1 again and factorizes the λ-term:

$$[-\lambda]^{-1/2-\epsilon} = [x_1^2(x_6^+ - x_6)(x_6 - x_6^-)]^{-1/2-\epsilon}$$
$$\to [\,y_6(1-y_6)\,]^{-1/2-\epsilon}[x_1(x_6^+ - x_6^-)]^{-1-2\epsilon}\,.$$

However, it is possible to eliminate the square roots by quadratic transformations, except in factors like $(1 - y_6^2)^{-1/2-\epsilon}$, which do not lead to singularities in ϵ and therefore are not subject to further sector decomposition. This nice feature will be spoiled in the $1 \to 5$ case.

The implementation of sector decomposition for the $1 \to 4$ phase space served for the calculation of all master phase space integrals which are needed for any $1 \to 4$ process in massless QCD. These master integrals have been derived and calculated analytically as well as numerically in [12].

Moreover, the method also can deal with the full matrix element without reduction to master integrals. This has been demonstrated in [16]. To split the calculation into smaller pieces, one can write the squared matrix element as a sum over different topologies. As the calculation is naturally parallelized by this subdivision into topologies, the overall runtime is given by the most difficult topology, which took about 9 hours for a precision of 0.1% and less than two hours for a precision of 1% on a Pentium IV 2.2 GHz PC.

3.2. $1 \to 5$ phase space

The $1 \to 5$ partonic phase space, relevant for the calculation of $e^+e^- \to 3\,\text{jets}$ at NNLO, in-

volves the integration over 9 independent invariants:

$$\int d\Phi_{1\to5} = C_\Gamma^{(5)} \int \prod_{j=1}^{10} dx_j \tag{5}$$

$$\delta(1 - \sum_{i=1}^{10} x_i) \, [\Delta_5(\vec{x})]^{(D-6)/2} \, \Theta(\Delta_5) \,.$$

Note that $C_\Gamma^{(5)} \sim V(D-4) = 2\pi^{-\epsilon}/\Gamma(-\epsilon)$ is of order ϵ, therefore the integral (5) contains a fake singularity in $[\Delta_5(\vec{x})]^{(D-6)/2} = [\Delta_5(\vec{x})]^{-1-\epsilon}$, but this presents no problem for sector decomposition as the algorithm will extract the singular factor and the ϵ-expansion subroutine will take the prefactor of order ϵ into account, such that the fake singularity will be eliminated automatically. What is more of a problem are the non-polynomial structures which occur here, because denominators of the form $g(x,y) = a + x + y - \sqrt{a^2 + x + y}$, where a is a constant, can produce a singularity for $x,y \to 0$ without having the right scaling behaviour amenable to sector decomposition. The task is to transform such terms away without increasing the complexity of the integrand too much. It should be noted that the size of the expressions in the $1 \to 5$ case is considerably larger than in the $1 \to 4$ case, such that it becomes much more important to produce as few subsectors as possible.

The simplest example to calculate is the 5-particle phase space volume without any matrix element. In [12] a general analytic expression for the $1 \to N$ phase space volume is given, such that the numerical result can be easily checked. By sector decomposition, one obtains

$$\int d\Phi_{1\to5} = \frac{(4\pi)^{4\epsilon-7}}{\Gamma(1-2\epsilon)\Gamma(2-2\epsilon)}\Big[0.00347$$
$$+0.05469\epsilon + 0.44336\epsilon^2$$
$$+2.47424\epsilon^3 + 10.7283\epsilon^4 + \mathcal{O}(\epsilon^5)\Big]$$

which agrees with the analytical result to an accuracy of 0.5% after a runtime of about 10 minutes.

3.3. One loop plus single real emission

Apart from the double real emission and the two-loop virtual contributions to the cross section of $e^+e^- \to jets$ at NNLO, there is also a contribution where one-loop virtual corrections are combined with single real emission. In this class, the most complicated diagram which can occur in the calculation of $e^+e^- \to 2\,$jets is a box graph with one off-shell leg. This type of diagram can easily be calculated by sector decomposition: The one-loop box can be expressed by Hypergeometric functions ${}_2F_1(1,-\epsilon,1-\epsilon;x_i/x_j)$. Then the parameter representation of the Hypergeometric functions can be used and the resulting one-dimensional parameter integrals can be combined with the ones for the 3-particle phase space to end up with a 4-dimensional parameter integral which can be directly fed into the sector decomposition routine.

For $e^+e^- \to 3\,$jets, the most complicated one-loop diagrams are pentagons with one off-shell leg. These could be reduced to boxes by standard reduction techniques [23,24], but as the reduction introduces inverse determinants of kinematic matrices which may lead to numerical instabilities, it is more convenient to apply the sector decomposition routine for loop integrals directly to the pentagon which is of the form

$$I_5 = -\Gamma(3+\epsilon) \int \prod_{i=1}^{5} dz_i \, \delta(1 - \sum_{i=1}^{5} z_i) \, \mathcal{F}^{3+\epsilon}$$
$$-\mathcal{F} = s_{12}\, z_1 z_5 + s_{23}\, z_1(z_3 + z_4 + z_5)$$
$$+ \quad s_{13}\, z_5(z_1 + z_2) + s_{14}\, z_5(z_1 + z_2 + z_3)$$
$$+ \quad s_{24}\, z_1(z_4 + z_5) + s_{34}\,(z_1 + z_2)(z_4 + z_5) \,.$$

After sector decomposition in the variables z_i, one obtains an expression where the poles of the virtual integral already have been extracted:

$$I_5 = \sum_{\alpha=0}^{2} P_\alpha/\epsilon^\alpha \,,$$

$$P_\alpha = \int_0^1 \prod_{i=1}^{4-\alpha} dt_i \, \mathcal{G}(t_i, s_{12}, \ldots, s_{34}) \,,$$
$$\lim_{t_i \to 0} \mathcal{G} \neq 0 \,.$$

This expression can then be inserted into the 4-particle phase space and one can proceed with decomposition in the scaled invariants $x_1, \ldots, x_6$. Note that no problems with thresholds will occur here as the kinematics is such that all invariants s_{ij} are non-negative.

4. SUMMARY AND OUTLOOK

The automated sector decomposition algorithm is a powerful method to isolate overlapping infrared poles and to calculate numerically not only multi-loop integrals, but also phase space integrals where some of the particles can become theoretically unresolved, leading to infrared singularities. In particular, the method allows the calculation of the one-loop plus single real emission and the double real emission contribution to $e^+e^- \to 2$ or 3 jets at NNLO without having to establish a subtraction scheme and to integrate analytically over complicated subtraction terms. The inclusion of a measurement function also does not present a problem, as has been demonstrated already in [17], such that a fully differential Monte Carlo program can be constructed based on this method. The only drawback of the method is the fact that it generates a large number of functions, but it has been shown already that in the case of $e^+e^- \to 2$ jets at NNLO, this does not lead to unacceptable integration times. Further, the functions are numerically well-behaved by construction. How the NNLO calculation of the process $e^+e^- \to 3$ jets with this method performs numerically will turn out in the near future.

The generalization to other processes than e^+e^- annihilation is feasible, but cases where some of the kinematic invariants take negative values cannot be treated without further development of the method.

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